A multiscale simulation technique for optimization of granular mixing

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Many industrial processes require manipulating granular materials, but simulation of these is challenging due to an incomplete picture of the underlying physics. Over the past decade, there has been a renewed scientific interest in this state of matter, that has revealed surprisingly complex behavior, such as fractal-like networks of force chains at the level of a single particle, which call into question the applicability of a general continuum model. So far there is no widely applicable model for an arbitrary granular flow, and most theories for flow have been limited to specific geometries.

For more complex questions, such as those about diffusion, mixing, and particle packing structure, there are very few models available. There is no thermal equilibrium in the conventional sense, so any particle rearrangement occurs only in response to outside forcing. Currently, questions about mixing in practical situations would typically be answered by using Discrete-Element Method (DEM) simulation. The contact models in these simulations are stiff and require very small timesteps to integrate accurately, meaning that even relatively small problems require days or weeks to run on a parallel computer [2]. These brute-force approaches are often infeasible for applications in real-time process control, or in optimization, where there is a need to run many different configurations much more rapidly.

In previous work, a multiscale simulation was demonstrated that was able to correctly capture diffusion and mixing in hopper drainage [1], by breaking down the flow into correlated group displacements on a mesoscopic length scale. In a related study, it was shown that continuum variables, while intractable at a level of a single particle, can successfully be interpreted at the same scale [3], and this information can be used to directly test and develop a continuum theory of granular materials.

Drawing on these concepts, a multiscale simulation technique will be presented, that couples a macroscopic continuum theory of granular flow to a discrete microscopic mechanism for particle motion. The technique can be applied to arbitrary slow, dense granular flows, and can reproduce similar packing statistics and diffusion estimates as in DEM. Since forces and stress are coarse-grained, the simulation technique runs two to three orders of magnitude faster than conventional DEM, which allows ensembles of simulations to be carried out in order to optimize mixing in a granular system.

References

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